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Finite-Temperature Phase Transition in the Montorsi-Rasetti Model.

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Abstract. – Exact diagonalization and quantum Monte Carlo methods are used to compute the specific heat and the charge and spin correlation functions for a two-dimensional system of correlated electrons, described by the Montorsi-Rasetti model. Our results strongly suggest the occurrence of an unusual phase transition at finite temperatures.

Recently, Montorsi and Rasetti (MR) introduced a modified Hubbard model [1-4]. The MR model describes a system of electrons which hop to nearest-neighbour lattice sites and which are coupled through a Coulomb interaction when two electrons of opposite spin occupy the same lattice site. Unlike in the Hubbard model, the nearest-neighbour hopping is occupation-dependent and does not conserve the spin. The Hamiltonian for the MR model is obtained from the Hamiltonian for the Hubbard model by including spin-flip hopping processes and hopping processes depending on the relative site occupation. Physically the former may be due to the presence of spin-orbit coupling [5] and the latter to the presence of a bond-charge interaction [6-9]. The MR Hamiltonian reads

$$\mathcal{H} = \frac{t}{2} \sum_{\langle i,j \rangle} \sum_{\sigma, \sigma'} (a_{i,\sigma}^\dagger a_{j,\sigma'} + \text{h.c.}) - \frac{\bar{t}}{2} \sum_{\langle i,j \rangle} \sum_{\sigma, \sigma'} (a_{i,\sigma}^\dagger a_{j,\sigma'} + \text{h.c.}) (n_{i,-\sigma} + n_{j,-\sigma'} - \gamma n_{i,-\sigma} n_{j,-\sigma'}) + U \sum_i n_{i,\uparrow} n_{i,\downarrow} - \mu \sum_i \sum_{\sigma} n_{i,\sigma}, \quad (1)$$

where $a_{i,\sigma}^\dagger$ and $a_{i,\sigma}$ are the creation and annihilation operators, respectively, for an electron with spin $\sigma = \uparrow, \downarrow$ at lattice site i , $n_{i,\sigma}$ denotes the number operator at site i , and the sum $\langle i,j \rangle$ is over distinct pairs of nearest-neighbour lattice sites on a d -dimensional hypercubic lattice of linear size L , t and \bar{t} are the hopping parameters, U the on-site Coulomb interaction, μ the chemical potential and γ a real number.

Numerical results, as obtained from exact diagonalization and Quantum Monte Carlo

(QMC), simulations showed that for dimensions $d = 1, 2, 3$ and $\gamma = 0, 2$ the MR model exhibits a Mott metal-insulator transition [10] at zero temperature as a function of U [11, 12]. At half-filling the metal-insulator transition occurs for $|U/4 dt| = 1$. For $|U/4 dt| < 1$ the system is a metal, otherwise it is an insulator. If the system is metallic there are ferromagnetic (FM) long-range (LRC) correlations in the x -component of the spin operator and in the charge distribution [12].

In this letter we present results for the specific heat and the temperature dependence of the magnetic and charge structure factors for the half-filled two-dimensional (2D) MR model for $|U/4 dt| < 1$. The results are obtained from exact diagonalization methods for lattices up to 16 sites and from QMC simulations for larger lattices. Our results strongly suggest that the FM LRC in the x -component of the spin operator and the charge distribution persist up to a critical temperature $T_c > 0$, signalling the occurrence of a magnetic and «charge» phase transition at T_c .

Following MR [1, 4] it is useful to rewrite Hamiltonian (1) as

$$\mathcal{H} = \sum_{i,j} A_i^\dagger M_{ij} A_j - \mu \sum_i D_i, \quad (2)$$

where $A_i = (a_{i,\uparrow} + a_{i,\downarrow})/\sqrt{2}$, $N_i = A_i^\dagger A_i$, $B_i = (a_{i,\uparrow} - a_{i,\downarrow})/\sqrt{2}$, and $D_i = B_i^\dagger B_i$. The matrix elements of M are given by $M_{ij} = UD_i - \mu$ if $i = j$, $M_{i,j} = t - \bar{t}(D_i + D_j - \gamma D_i D_j)$ if i and j are nearest neighbours and $M_{ij} = 0$ otherwise.

From (2) it is clear that the MR model can be interpreted as 1) a model for mixed-valence states in rare-earth compounds, *i.e.* an extended spinless symmetric Falicov-Kimball model [13], where the moving particles (A_i 's) play the role of s -electrons and the localized ones (B_i 's) stand for the f -electrons, 2) a model for an annealed binary alloy or for crystallization [14, 15] in which the electrons are described by the A_i 's and the ions by the B_i 's, and 3) the simplified Hirsch model, *i.e.* the one obtained by applying to the Hirsch model [16] Hubbard's approximation [17] of localizing one of the spin species.

As all D_i commute with all A_i and A_i^\dagger , it follows immediately that the grand canonical partition function can be written as

$$Z \equiv Z(t, U, \mu, \gamma) = \sum_{\{s_i = 0, 1\}} \exp \left[\beta \mu \sum_i s_i \right] \text{tr} \exp \left[-\beta \sum_{i,j} A_i^\dagger M_{ij}(\{s_i\}) A_j \right], \quad (3)$$

where $M_{ij}(\{s_i\})$ is given by M_{ij} with D_i replaced by s_i , the eigenvalues of the operators D_i , and tr denotes the trace over the spinless fermions A_i . Because $\mathcal{H}(\{s_i\})$ is a quadratic form in the A_i 's, the trace over the $n_i = 0, 1$'s can be performed analytically, yielding for the partition function the exact expression

$$Z = \sum_{\{s_i = 0, 1\}} \det [1 + \exp[-\beta M(\{s_i\})]] \exp \left[\beta \mu \sum_i s_i \right]. \quad (4)$$

In contrast to the expression for Z one obtains for the Hubbard model [18], the determinant in (4) is strictly positive. This ensures that there will be no minus-sign problems in the Monte Carlo simulations [18].

Expression (3) is a convenient starting point to discuss the symmetry properties of the Hamiltonian that are relevant for the description of the phase transition. For the sake of brevity we only consider the case $\bar{t} = t$ in the following. First, if A_i is replaced by $(1 - 2D_i)A_i$ on all odd numbered sites of a hypercubic lattice, then $Z(t, U, \mu, \gamma) = Z(t, U, \mu, 2 - \gamma)$, showing that the thermodynamic properties for $\gamma = 0, 2$ are the same. Second, interchanging particles and holes for the A fermions, *i.e.* replacing A_i^\dagger by A_i and N_i by $1 - N_i$, gives $Z(t, -U, -\mu, \gamma) = \exp[-\beta \mu L^d] Z(t, U, \mu, \gamma)$ for $U = 2\mu$. Third, if particles and holes are

interchanged for the A fermions as well as for the B fermions then $Z(t, U, U - \mu, \gamma) = \exp[-\beta(2\mu - U)L^d]Z(t, U, \mu, \gamma)$ for $\gamma = 0, 2$, and if, in addition, $U = 2\mu$ the partition function remains unchanged. It then follows that for $\gamma = 0, 2$ and $\mu = U/2$, $L^{-d} \sum_i \langle D_i \rangle = 1 - L^{-d} \sum_i \langle D_i \rangle$ and analogously for N_i , so that $L^{-d} \sum_i \langle D_i \rangle = L^{-d} \sum_i \langle N_i \rangle = 1/2$. As a consequence, the electron density $n = L^{-d} \sum_i \langle D_i + N_i \rangle = 1$, i.e. the band is half-filled.

Exact expression (1) for the partition function can also be written as $Z = \sum_{\{s_i=0,1\}} \exp[-\beta E(\{s_i\})]$, with $E(\{s_i\}) = -\beta^{-1} \ln \det(1 + \exp[-\beta M(\{s_i\})]) - \mu \sum_i s_i$, showing that the MR model can be viewed as a classical lattice gas (Ising) model with peculiar interactions. Indeed, M contains on-site and nearest-neighbour couplings only but $\exp[-\beta M(\{s_i\})]$ is highly non-local. Furthermore, from the definition of the determinant it follows immediately that the effective interaction between the variables s_i is extremely complicated. Nevertheless an approximate mapping onto the 2D Ising model can be constructed as follows. For $\gamma = 2$ and a half-filled band ($U = 2\mu$) Hamiltonian (2) can be written as

$$\mathcal{H} = \frac{t}{2} \sum_{(i,j)} A_i^\dagger (1 + \sigma_i \sigma_j) A_j + \frac{U}{2} \sum_i \left(N_i - \frac{1}{2} \right) \sigma_i - \frac{UL^2}{4}, \quad (5)$$

where (i, j) runs over all pairs of nearest-neighbour lattice sites and $\sigma_i = \pm 1$ are Ising variables. A rigorous lower bound to Z is obtained by applying inequality $\text{tr} \exp[-\beta \mathcal{H}]/\text{tr} \exp[-\beta \mathcal{H}_0] = \text{tr} \exp[-\beta \mathcal{H}_0] \exp[\beta \mathcal{H}_0] \exp[-\beta \mathcal{H}]/\text{tr} \exp[-\beta \mathcal{H}_0] = \langle \exp[\beta \mathcal{H}_0] \exp[-\beta \mathcal{H}] \rangle_0 \geq \exp[\beta \langle \mathcal{H}_0 - \mathcal{H} \rangle_0]$, with $\mathcal{H}_0 = (t'/2) \sum_{(i,j)} A_i^\dagger A_j$ (¹), yielding

$$Z \geq \exp[\beta UL^2/4] \exp[\beta(1 - t/t')E_0(\beta)] (\text{tr} \exp[-\beta \mathcal{H}_0]) \sum_{\{\sigma_i = \pm 1\}} \exp\left[-\frac{\beta E_0 t(\beta)}{2L^2 t'} \sum_{(i,j)} \sigma_i \sigma_j\right], \quad (6)$$

where $E_0(\beta) \equiv \langle \mathcal{H}_0 \rangle_0$ is the free-particle energy. The third factor of the r.h.s. of (6), being the partition function of the 2D Ising model, exhibits a singularity at the inverse temperature β^* given by the solution of $-t\beta^* E_0(\beta^*) T_c^{(1)} = 2L^2 t'$, where $T_c^{(1)} \approx 2.27$ is the critical temperature of the 2D Ising model on a square lattice. An order of magnitude estimate of β^* is obtained by replacing $E_0(\beta^*)/L^2$ by its ground-state value of the infinite system $\lim_{L \rightarrow \infty} \lim_{\beta \rightarrow \infty} E_0(\beta)/L^2 t' = -4/\pi^2$, yielding

$$T^*/t \approx \frac{T_c^{(1)}}{\pi^2} \approx 0.47, \quad (7)$$

independent of U and t' . Note that, although the lower bound (5) exhibits a phase transition of the Ising type, it does not follow from (5) that Z should also display a singularity as a function of temperature.

To explore the occurrence of a finite-temperature phase transition in the metallic regime of the half-filled 2D MR model ($|U/t| < 8$), we first consider the behaviour of the specific heat as a function of temperature. The specific heat is calculated according to its explicit grand canonical ensemble expression given in ref. [7]. For $|U/t| < 8$, the numerical results reveal a narrow peak at low and a broad one at higher temperatures. The broad peak, which turns out to be rather independent of the system size, might be attributed to single-particle excitations from the lower to the upper band in the density of states. As seen in fig. 1, for

(¹) This inequality also holds if $[H_0, H] \neq 0$.

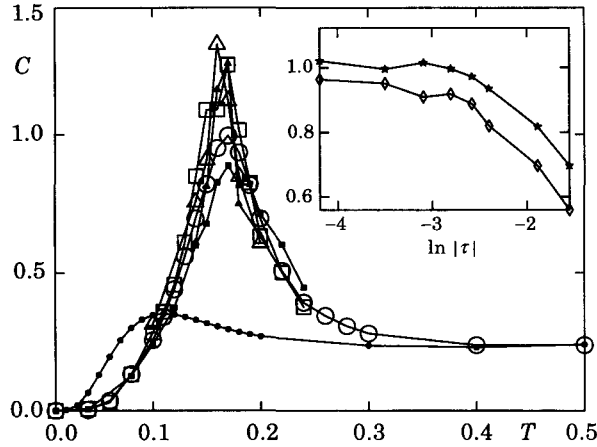


Fig. 1. – Specific heat per site as a function of temperature for half-filled 2D lattices for $\tilde{t} = t = 1$, $\gamma = 2$ and $|U/t| = 4$. ●: exact results for a 4×4 lattice; ■: QMC data for a 6×6 lattice; ○: QMC data for a 8×8 lattice; □: QMC data for a 10×10 lattice; ▲: QMC data for a 12×12 lattice; △: QMC data for a 14×14 lattice. The lines are guides to the eye. Inset: specific heat as a function of $\ln |\tau|$, $\tau = 1 - T/T_c$, for a half-filled 8×8 lattice for $\tilde{t} = t = 1$, $\gamma = 2$, $|U/t| = 4$ and $T_c = 0.165$. ★: $T > T_c$; ◇: $T < T_c$. The lines are guides to the eye.

$|U/t| = 4$ the height of the sharp peak occurring around $T = 0.165$ depends on system size and with that, points to the occurrence of a phase transition associated with charge and spin ordering. The weak size dependence suggests a singularity of the form $C = \alpha^{-1} A^\pm |\tau|^{-\alpha}$ with $\alpha \approx 0$, $\tau = 1 - T/T_c$ and the critical amplitudes A^+ and A^- above and below T_c , respectively. To substantiate the small value of α , we included in fig. 1 a plot of C vs. $\ln |\tau|$ with $T_c = 0.165|t|$, because for α small: $C = \alpha^{-1} A^\pm |\tau|^{-\alpha} = \alpha^{-1} A^\pm \exp[-\alpha \ln |\tau|] \approx \alpha^{-1} A^\pm - A^\pm \ln |\tau|$. For this value of T_c the data is seen to fall on two nearly parallel branches, indicating $A^+/A^- \approx 1$. In this plot, the bending and the saturation of the specific heat for small τ -values must be attributed to the finite size. Nevertheless, this data provides considerable evidence for the occurrence of a phase transition close to $T_c = 0.165|t|$ with $\alpha \approx 0$.

Additional calculations (not shown) for other values of $|U/t| < 8$ indicate that T_c reaches a maximum for $U = 0$ and decreases with $|U|$. For $U = 0$, $T_c \approx 0.25|t|$ in reasonable agreement with the rough estimate (7).

To substantiate the phase transition further we have studied the temperature dependence of the distribution of charges and magnetic moments in the system. The relevant quantities to study are the charge density correlation function

$$C_D(q) = \frac{1}{L^2} \sum_{j,k} \exp[iq(j-k)] (\langle (N_j + D_j)(N_k + D_k) \rangle - \langle N_j + D_j \rangle \langle N_k + D_k \rangle), \quad (8)$$

and the spin density correlation function

$$S_D^{(\nu)}(q) = \frac{1}{L^2} \sum_{j,k} \exp[iq(j-k)] (\langle S_j^{(\nu)} S_k^{(\nu)} \rangle - \langle S_j^{(\nu)} \rangle \langle S_k^{(\nu)} \rangle), \quad \nu = x, y, z, \quad (9)$$

where $S_j^{(\nu)}$ denote the spin operators at site j and are given by $S_j^{(\nu)} = \sum_{\sigma, \sigma'} a_{j, \sigma}^\dagger \alpha_{\sigma \sigma'}^{(\nu)} a_{j, \sigma'}$, where $\alpha_{\sigma \sigma'}^{(\nu)}$ are the Pauli spin matrices. For the MR model, because of the presence of spin-flip

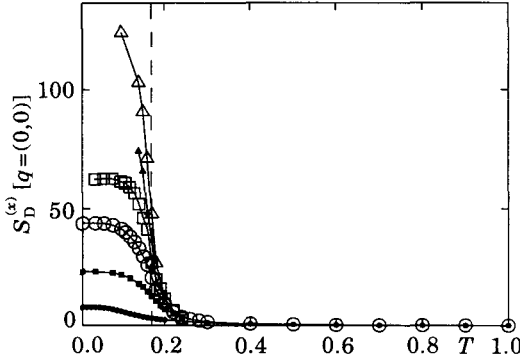


Fig. 2.

Fig. 2. – Spin density correlation function $S_D^{(x)}(q = (0, 0))$ as a function of temperature for half-filled 2D lattices for $\bar{t} = t = 1$, $\gamma = 2$ and $U/t = 4$. ●: exact results for a 4×4 lattice; ■: QMC data for a 6×6 lattice; ○: QMC data for a 8×8 lattice; □: QMC data for a 10×10 lattice; ▲: QMC data for a 12×12 lattice; △: QMC data for a 14×14 lattice. Dashed line: estimated value of T_c . The lines are guides to the eye.

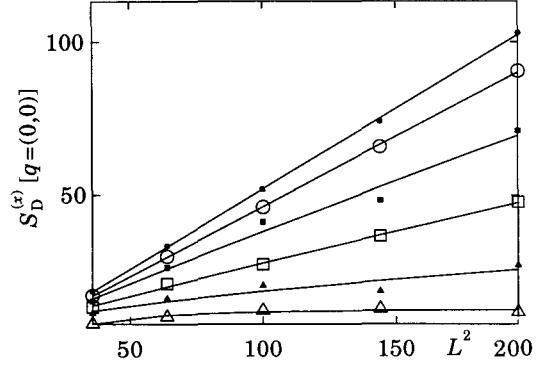


Fig. 3.

Fig. 3. – Spin density correlation function $S_D^{(x)}(q = (0, 0))$ as a function of L^2 for half-filled 2D lattices for $\bar{t} = t = 1$, $\gamma = 2$ and $U/t = 4$. ●: $T = 0.14$; ○: $T = 0.15$; ■: $T = 0.16$; □: $T = 0.17$; ▲: $T = 0.18$; △: $T = 0.2$. The lines are best fits through the data points.

hopping processes, only the expectation value of the x -component of the spin operator $\sum_j \langle S_j^{(x)} \rangle = \sum_j \langle N_j - D_j \rangle$ may be non-zero. At half-filling $\sum_j \langle S_j^{(x)} \rangle = 0$ because $\sum_j \langle N_j \rangle = \sum_j \langle D_j \rangle = 1/2$. Furthermore, only the x -component of the spin operator at site j is correlated with the x -component of the spin operator at site k , whereas all correlation functions for the y and z components are zero [12]. At half-filling it follows from particle-hole symmetry applied to the A -fermions that, on reversing the sign of U , $S_D^{(x)}(q)$ and $C_D(q)$ interchange (see (7)).

Figure 2 shows the $q = (0, 0)$ spin correlation function $S_D^{(x)}(q = (0, 0))$ for $U/t = 4$ as a function of temperature for half-filled 2D lattices of various size. For temperatures well above $0.17|t|$, $S_D^{(x)}(q = (0, 0))$ is independent of the lattice size. At low temperatures the data is consistent with $S_D^{(x)}(q = (0, 0)) \propto L^2$ and similar behaviour was found for the charge correlation function $C_D(q = (0, 0))$. Since $\langle S_i^{(x)} \rangle = 0$ for all T and since for $T < T_c$ the correlation length in a finite system is proportional to the linear size L , this behaviour suggests long-range spin and charge correlations for all temperatures below T_c . At $T_c \approx 0.165|t|$ the data shown in fig. 3 is consistent with $S_D^{(x)}(q = (0, 0)) \propto L^2$. Standard finite-size scaling [19] implies for the correlation function $S_D^{(x)}(q) \propto q^{\gamma-2} \propto L^{2-\gamma}$ for $q \rightarrow (0, 0)$, $\gamma \approx 0$ and, with the scaling relation $\gamma = \nu(2 - \gamma)$, $\gamma = 2\nu$. Together with the hyperscaling relation $d\nu = 2 - \alpha$ and $\gamma + 2\beta + \alpha = 2$, our estimate for the specific-heat component, $\alpha \approx 0$, implies $\gamma \approx 2$, $\nu \approx 1$ and $\beta \approx 0$. In this context we note that our estimates for T_c , γ and ν are in good agreement with the finite-size scaling expression [20, 21]

$$S_D^{(x)}(q = (0, 0), T) = L^{\gamma/\nu} G(L^{1/\nu} |T - T_c| T_c^{-1}), \quad (10)$$

in terms of the resulting collapse of the data towards the universal scaling function G .

Thus, our analysis strongly suggests that the MR model exhibits a phase transition characterized by a vanishing expectation value of the order parameter and long-ranged

correlations below and at the critical temperature. In this respect there is some similarity to the Kosterlitz-Thouless phase transition in the 2D-XY-model. Our estimates for the critical exponents, however, point to rather different and novel critical behaviour.

* * *

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REFERENCES

- [1] MONTORSI A. and RASETTI M., *Phys. Rev. Lett.*, **66** (1991) 1383.
- [2] MONTORSI A. and RASETTI M., *Int. J. Mod. Phys. B*, **5** (1991) 985.
- [3] MONTORSI A. and RASETTI M., *The Hubbard Model: Recent Results*, edited by M. RASETTI (World Scientific, Singapore) 1991.
- [4] MONTORSI A. and RASETTI M., *Microscopic Aspects of Non-linearity in Condensed Matter*, edited by A. R. BISHOP, V. L. POKROVSKY and V. TOGNETTI (Plenum, New York, N.Y.) 1991.
- [5] FRIEDEL J., LENGHART P. and LEMAN G., *J. Phys. Chem. Solids*, **25** (1964) 781.
- [6] KIVELSON S., SU W.-P., SCHRIEFFER J. R. and HEEGER A. J., *Phys. Rev. Lett.*, **58** (1987) 1899.
- [7] BAERISWYL D., HORSCH P. and MAKI K., *Phys. Rev. Lett.*, **60** (1988) 70.
- [8] GAMMEL J. T. and CAMPBELL D. K., *Phys. Rev. Lett.*, **60** (1988) 71.
- [9] KIVELSON S., SU W.-P., SCHRIEFFER J. R. and HEEGER A. J., *Phys. Rev. Lett.*, **60** (1988) 72.
- [10] MOTT N. F., *Metal-Insulator Transitions* (Taylor and Francis, London) 1974.
- [11] MICHIELSEN K., DE RAEDT H. and SCHNEIDER T., *Phys. Rev. Lett.*, **68** (1992) 1410.
- [12] MICHIELSEN K., *Int. J. Mod. Phys. B*, **7** (1993) 2571.
- [13] FALICOV L. M. and KIMBALL J. C., *Phys. Rev. Lett.*, **22** (1969) 997.
- [14] KENNEDY T. and LIEB E. H., *Physica A*, **138** (1986) 320.
- [15] JEDRZEJEWSKI J., LACH J. and LYZWA R., *Physica A*, **154** (1989) 529.
- [16] HIRSCH J. E., *Physica C*, **158** (1989) 326.
- [17] HUBBARD J., *Proc. R. Soc. London, Ser. A*, **276** (1963) 238.
- [18] DE RAEDT H. and VON DER LINDEN W., *The Monte Carlo Method in Condensed Matter Physics*, edited by K. BINDER, *Topics in Applied Physics*, **71** (Springer, Berlin) 1992.
- [19] FISHER M. E., *Rev. Mod. Phys.*, **46** (1974) 597.
- [20] FERDINAND A. E. and FISHER M. E., *Phys. Rev.*, **185** (1969) 832.
- [21] FISHER M. E. and FERDINAND A. E., *Phys. Rev. Lett.*, **19** (1967) 169.